Role of a magnetism in a stability of CoCrFeMnNi and its devivates

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Abstract

Multi-principal elements alloys, called as 'High Entopy Alloys', represent a promising group of materials, due to its possible applications in the industry. They form a single phase solid solution based on high number of components in near-equimolar composition, that often brings a high entropy contribution to the Gibbs free energy. It is considered as the main contribution stabilizing the alloy at higher temperatures. In the current work we'd like to focus on another contributions, which could affect stability of the system, i.e magnetic interactions among all atoms. Using ab-initio calculations based on TB-LMTO-ASA within CPA we studied the stability of the well known 'Cantor alloy' CoCrFeMnNi as well as related phases with a nonmagnetic substitution were calculated. For a similar reason non-homogeneous structures and magnetic exchange interactions were studied as well. We report strenghts of the mutual interactions between the elements and their impacts on the stability of the alloy. Further we discuss the importance of mutual exchange ineraction and its contribution to the final preferred magnetic ordering of studied phase. Finally we suggest possible way for stabilizing the parent structure.

Keywords: HEA, DFT, enthalpy, magnetism, exchange inteactions
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1. Introduction

High entropy alloys (HEA), whose research and development commence in the beginning of the century seem to be a group with extraordinary properties promising wide range of applications. There are mentioned several of them as mechanical properties: high hardness [1], extreme tensile strength [2], great fatigue resistance [3]. Also distinct electrical properties were reported e.g an anomalous Hall effect [4], Kondo-like behavior [5] or a low-temperature superconductivity [6] and more others examples can be found in literature. The HEAs are so-called multi-principal element alloy based on several chemical element unlike standard alloys as a steel.

There exist a few criterion defining HEAs, which represents distinct definitions of HEAs. Firstly they are composed of at least five principal elements in a nearly equimolar ratio, where the concentration of principal elements stay in the range between 5-35 % [7–9]. Further constrains on the total configuration entropy S_{conf} are stated. Alloys are divided in low, medium and high entropy alloy with $S_{conf} > 1.61R$ (R is the molar gas constant), which is much higher than for conventional alloys [8–10]. Such high configuration entropy is reach in case of five principal element for the equimolar composition, but also quaternary alloy with much lower configuration entropy are considered as HEAs [11]. Hence a new entropy limit is suggested $S_{conf} = 1.5R$ [7, 12]. Finally single phase solid solutions for HEAs is required. Solid solution don't exhibit long range chemical ordering like intermetalic compound with distinguished chemical sub-lattices. Only short range chemical ordering could appear [8].

High values of configuration entropy S_{conf} in concepts of HEAs are demanded due to the stabilization solid solution phase. For a sufficiently high temperature the entropic term ($-TS$, T is the temperature) can overcame the formation enthalpy H_{form} in the definition of Gibbs free energy G and favor the solid solution phase instead of an intermetallic phase [7, 9, 13]. It is important to point out that a high entropy doesn't guaranty existence of solid solution phase and not only solid

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solution phase are presented in HEAs [9].

Among the other the most studied HEAs are alloys based on 3d elements [8]. Well known HEA belonging to this group is the ‘Cantor alloy’ CoCrFeMnNi [14] with a FCC single solution phase. It is one of a primal and model HEAs, which exhibit exceptional ductility and toughness at low temperatures [15, 16].

In a present work we are focusing on the ab-initio calculations of the ‘Cantor’ alloys and its derivates. We are interested in the ground state magnetic structure and magnetic interaction in this compound. Since we are also dealing with a non-magnetic substitution to obtain deeper inside view in their properties,

2. Methods

Calculation were performed by using tight-binding linear muffin-tin method based on the Green’s function formalism within the atomic sphere approximation [17, 18] (TB-LMTO-ASA). The local spin density approximation with Vosko-Wilk-Nursair exchange potential [19] and s, p, d atomic model were involved. The method offers calculation of band structure in scalar relativistic approximation where the on-site spin-orbit coupling is add to scalar relativistic hamiltonian or in fully relativistic way solving Dirac equation in relativistic formalism [18]. To improve solving electrostatics in disorder system a basic screened impurity model were incorporated [20]. The advantage of this approach consist in solving chemically disorder in solids, because of straightforward implementation single-site coherent potential approximation (CPA). It is especially suitable for treating small perturbation as small concentration or similar atoms, which is the case of ”CoCrFeMnNi”. It’s a computationally efficient method, because instead of large supercells only small number of atomic sites is sufficient. For a simple ferromagnetic FCC cell only single site is needed. More complicated magnetic ordering as antiferemagnetic or non-collinear required a increased number of sites

In the construction of the elemental cell various atomic radii were used based on their metallic radii [21]. Actually the prescribed rations between them had to be fulfilled as the cell volume change. Then the lattice relaxation of parameters were done by changing a lattice parameter followed by a appropriate change of atomic radii, where a energetic dependence were evaluated. Obtaining the calculated electron structure there is a way to calculate the exchange interaction thanks to the used green formalism by the Liechtenstein formula, where the LMTO potential parameters and averaged Green’s function were employed. The electron structure calculations were mainly performed in full relativistic method. Due to implementation of the Liechtenstein formula result obtained in the scalar relativistic approximation were used as inputs for calculating exchange interactions. Observed differences between both approached will be discussed.

3. Results and Discussion

3.1. Ground state, Magnetic properties

In order to evaluate the formation enthalpy H_{form} of CoCrFeMnNi and its derivatives the energetic ground states of pure elements were found by a lattice parameter optimalization. Elements with following lattice type and magnetic structures were chosen. A non-magnetic BCC molybdenum and ferromagnetic ordered HCP cobalt, BCC iron and FCC nickel were calculated. The obtained lattice parameters almost well correspond to the experimentally measured ones **citace** (Tab. 1). Magnitudes of Co, Fe and Co moments fit well to the experimental values [22–24]. Contrary magnitudes of the other magnetic moments are significantly suppressed compared to the experimental results [25, 26] (Tab. 1). Partly it is likely consequence of used method. It doesn’t offer lattice relaxation as another approach due to unavailable interatomic forces. Hence discrepancies should can consist in a magneto-volume effect [18, 27]. Besides chromium and manganese have complicated magnetic structures. Spin density waves and a non-collinear magnetism appears there [28–30]. In case of manganese the antiferromagnetic (AFM) BCC structure with two atomic sites were selected as a initial magnetic structure. Probably due to the natural complex magnetic structure an underestimated lattice parameter were obtained compared to the experimental value [25]. It also influence the magnitude of a magnetic moment, because the calculated values dramatically vary with changing lattice size, which correspond with discrepancies in their reported calculated values. They strongly depends of used method and selected lattice form [31]. Also experimental values are not uniform. For a simple AFM bcc model they vary in range (1.35-2.83) μ_{B} [31] Lattice parameters in (Tab. 1) belong to the complex BCC structure with 58 atoms. The chromium did not converge to a magnetic state and gives a roughly zero magnetic moments. For a comparison in the literature value between (0.4-0.8) μ_{B} can be found [30]. Nevertheless the obtained lattice parameters fits quite well to the experimental one [26]. In a comparison they are only slightly under estimated.

	lattice type	magnetic phase	magnetic moment (μ_B)	lattice parameter (Å)
Co	hcp	FM	1.60 (1.57)	2.46 (2.51)
Cr	bcc	AFM	~ 0 (0.4-0.8)	2.82 (2.88)
Fe	bcc	FM	2.15 (2.26)	2.80 (2.87)
Mn	bcc	AFM	0.87 (1.35-2.83)	8.42 (8.88)
Ni	fcc	FM	0.66 (0.61)	3.48 (3.52)
Mo	bcc	NM	-	3.18 (3.15)

Table 1: Calculated lattice parameters and magnetic moments for selected elements. **pridat reference** Mn lat.[25]
Cr [26] Co [32]

Hence one can assume that the appropriate energies obtained for the AFM system should be somehow overestimated, since the proper magnetic configuration were not reached. It leads to deviation in determining of formation enthalpy H_{form} and evaluation of the stability of a studied system.

For the 'Cantor alloy' and its derivatives basic magnetic ordering phases (non-magnetic NM, ferrromagnetic FM, anti-ferromagnetic AFM) were calculated. Also more complicated structure were studied. The paramagnetic state with diluted magnetic moments (DLM) were simulated and a kind of non-collinear magnetic structures with a possible fluctuation of spin amplitude as well. We will denote it as spin density wave (SDW). Due to the presence of FCC lattice it was chosen structure, where the magnetic spins rotated along the [111] direction, which respect the close packing structure of FCC lattice. The Wigner-Seitz radii of the atoms were chosen as their metallic radii [33]. Using of differentiate atomic radii is important due to their effect on the total energy, lattice parameters and magnetic moments. We checked that differences in atomic radii can not be neglected.

3.1.1. CoCrFeMnNi - 'Cantor Alloy'

Initially we studied the parent Cantor alloy, primarily within a FCC structure, which is experimentally reported [14, 34].

We found out that for a simple FCC structure the Cantor alloy prefers paramagnetic state (Fig. 1) with tiny diluted magnetic moments (Tab. 2). The obtained value of the equilibrium lattice parameter ($a = 3.48$ Å) is comparable to the experimental values [14, 34, 35].

Noticeable magnetic moments were obtain for a more complicated non-collinear SDW structure described above, which indicates that the alloy likely tends to a non-collinear magnetic structure. The CoCrFeMnNi alloy in SDW phase shows a ferrimagnetic ordering in each layer of simulated system with anti-parallel ordered Co, Fe, Ni on the one hand and Cr, Mo on the other hand. In the text a ferrimagnetic phase is in general denoted as FM since composing of a single magnetic sublattice with collinear moments. A ferrimagnetic ordering within a single layer is supported by the antiparallel behavior which was describer in CoCrFeMnNi [34] with similar directions and magnitudes of magnetic moments and in CoCrFeNi alloy [36] as well. In general it was said that Cr and Mn are elements with a complicated magnetic structure, where an anti-parallel alignment appears. Hence a ferrimagnetic structure caused by such elements is not surprising. And also they might cause suppression of magnetic moments for a collinear magnetic structures.

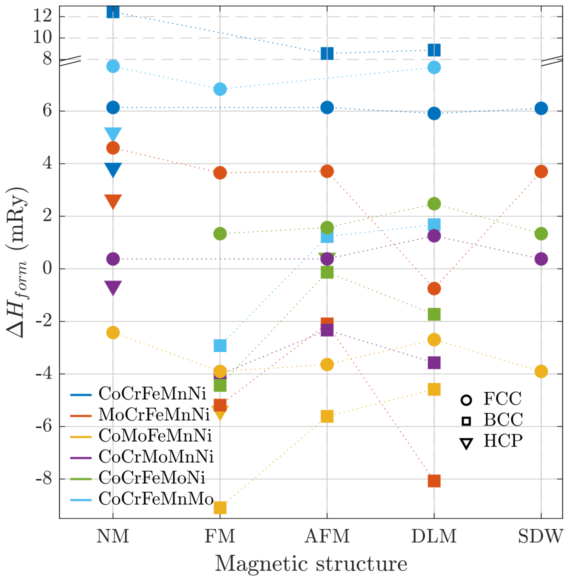

Figure 1: Configuration enthalpy for studied CoCrFeMnNi and derivatives dependent on the magnetic structure.

The calculated formation entropies H_{form} (Fig. 1) do not describes exactly the stability of studied alloys, since other effect are could be presented there. One can mention configuration entropy, entropy of vibrations etc. [37]. They can only some how represent the low temperature properties no the ambient one. Also it has to be point out that only simple lattice relaxation were used. Differences between calculated and real values of lattice parameters can consist in magneto-volume effect and in the fact that the calculated ones represent ground state properties at zero temperature. On the other hand they lies in the range of reported results obtained by different approach [37–39]. Obtained magnitudes of magnetic moments correspond well to reported

lattice		FCC						BCC						HCP					
alloy	magnetic structure	lattice param. (Å)	magnetic moments per element (μ_B)					lattice param. (Å)	magnetic moments per element (μ_B)					lattice param. (Å)	magnetic moments per element (μ_B)				
CoCrFeMnNi	FM	3.48	~ 0					2.75	~ 0					2.46	~ 0				
	AFM	3.48	-0.01	0.00	0.20	-0.01	0.00	2.80	-1.31	0.66	2.07	1.73	-0.27						
	DLM	3.48	0.02	0.00	0.11	0.06	0.00	2.79	1.01	0.00	2.03	1.00	0.00						
	SDW	3.49	0.16	-0.11	0.82	-0.17	0.06												
MoCrFeMnNi	FM	3.62	-0.04	-0.12	1.09	-0.22	0.04	2.88	-0.12	-0.21	2.06	1.38	0.20	2.55	~ 0				
	AFM	3.62	0.00	0.02	1.01	0.14	0.00	2.87	-0.09	0.13	1.84	0.60	-0.07						
	DLM	3.62	0.00	0.00	0.98	0.17	0.00	2.88	0.00	0.00	2.00	1.09	0.00						
	SDW	3.61	-0.03	-0.11	0.99	-0.18	0.03												
CoMoFeMnNi	FM	3.58	0.48	-0.05	1.53	-0.78	0.10	2.87	1.44	-0.19	2.22	1.92	0.30	2.53	0.27	-0.05	0.78	-0.34	0.38
	AFM	3.59	-0.09	0.01	1.33	0.76	-0.01	(2.89)	-1.30	0.20	2.18	2.20	0.24						
	DLM	3.58	0.00	0.00	1.28	-0.65	0.00	2.87	0.91	0.00	2.12	1.87	0.00						
	SDW	3.59	0.48	-0.05	1.53	-0.78	0.10												
CoCrMoMnNi	NM	3.61	~ 0					2.87	-0.80	-0.20	-0.04	1.00	0.07	2.55	~ 0				
	AFM	3.61	0.00	0.00	0.00	0.04	0.00	2.86	0.88	0.21	0.06	0.94	-0.20						
	DLM	3.61	-0.01	0.00	0.00	0.12	0.00	2.87	0.92	0.00	0.00	1.44	0.00						
	SDW	3.59	~ 0																
CoCrFeMoNi	FM	3.61	0.48	-0.28	1.46	-0.08	0.11	2.87	1.28	0.06	2.14	-0.06	0.13						
	AFM	3.60	-0.03	0.01	1.20	0.00	0.00	2.85	0.62	0.03	1.84	0.06	-0.09	2.54	0.00	0.00	0.04	0.00	0.00
	DLM	3.60	0.00	0.00	1.21	0.00	0.00	2.87	0.87	0.00	2.04	0.00	0.00						
	SDW	3.61	0.48	-0.28	1.46	-0.08	0.11												
CoCrFeMnMo	FM	3.60	0.10	-0.10	0.86	-0.14	-0.03	2.89	1.48	-0.03	2.18	1.71	-0.11	2.55	~ 0				
	AFM		not converged					(2.87)	-1.20	0.907	1.83	1.94	0.22						
	DLM	3.61	0.03	0.00	0.86	0.19	0.00	2.88	1.04	0.00	2.05	1.08	0.00						
	SDW		not converged																
CoMoFeMoNi	FM	3.70	0.64	-0.11	1.75	-0.11	0.12	-						-					

Table 2: Calculated lattice parameters and magnetic moments for CoCrFeMnNi and its derivatives depending on the lattice and magnetic structure. Results obtained from fully relativistic calculations.

ones [37]. Energetic difference to other magnetic structures for FCC structure is quite small. Hence it might not be in the contrary of observed spin-glass and ferromagnetic phase in low temperature [34]. The high temperature paramagnetic phase is also reported in other sources e.g. [40, 41].

For a thoroughgoing analysis we perform calculation for a BCC and HCP crystal structure in addition. They revealed that HCP structure is more stable in a ground state, which is in accordance with other studies [37]. It doesn't deny that FCC structure is a high temperature phase due to relatively small energetically difference.

3.1.2. Mo - derivatives

To clarify the magnetic behavior in this alloy it is worthy to study derivatives of the parent CoCrFeMnNi besides. For this purpose a nonmagnetic molybdenum substitution in a FCC CoCrFeMnNi, where all atoms are in principal magnetic, were used. They were calculated in a FCC structure, which is suitable for comparison with parent Cantor alloy and in a BCC structure reflecting their real structure [42] (besides HCP structure were checked to confirm a ground state configuration). The optimized lattice parameters, obtained magnitudes of magnetic moments and the formation enthalpy are presented in (Tab. 2) and (Fig. 1) Their behavior in BCC and FCC phase considerably differs.

For a BCC structure a collinear ferrimagnetic structure prevails. It gives large magnetic moments on Co, Fe and Mn atoms, which are almost parallely ordered. Tiny moments appears on Ni and Cr with an anti-parallel direction. One can notice that, the most important elements for magnetic ordering seems to be Fe and Co. The absence of Fe atoms leads to the large suppression of magnetic moments and a change of their direction compared to other derivatives. It shows that the directions are driven by Fe magnetic moments. The substitution of Co brings a paramagnetic DLM phase favorable only in this case. It is accompanied by smaller Mn and Fe magnetic moments An interplay between Cr and Mn was observed, while they are substituted. The magnitudes of their magnetic moments become more positive when the other element disappear (Tab. 2). Calculating the formation enthalpy we found out that the most stable derivative from this point of view is the alloy with substituted Cr atoms. One can notice that it gives the highest values of magnetic moments, an induced Mo moment included. It is follow by paramagnetic derivative with substituted Co and ferrimagnetic one related to the Mn substitution.

A FCC structure leads in all cases to strong suppression of magnetic moments, but mostly the behavior remain unchanged. The most stable form on substitution from our calculation stays the case of substituted Cr atom giving FM phase. It is followed by paramagnetic phase for substituted cobalt atoms and then again the FM phase for a substituted Mn atoms. This is exactly the same as in the previous structure. Fe atoms are still the most important element for establishing magnetism. Moreover it doesn't exist without their presence. A stable collinear FM phase appears only in case on a substitution of Cr or Mn, alternatively both of them. It indicates that the antiferomagnetic elements as Cr and Mn are probably obstacle for a magnetic state there. It is pronounce in increasing of magnetic moments compared to SDW phase of parent alloys with FM phases while Cr or Mn atoms are substituted. Another substitution, which reduced formation enthalpy H_{form} tends non-magnetic or paramagnetic DLM state. One can notice that chromium and manganese express their mutual antipathy in the magnitude of magnetic moments (Fig. 2) and for FM phase they always form a magnetic sublattice anti-parallel to the other elements. A similar indication was observed in the BCC structure. The above mentioned paramagnetic DLM state appears in the MoCrFeMnNi alloy for both structures. It may indicates an importance of Co for a magnetic behavior. Still it doesn't cause significant changes of magnetic moments in the FCC structure. Finally it was observed that Ni has no significant effect on the evolution of magnetic moments. Further its absence gives a FM state, but it leads to increasing of formation enthalpy.

At the end we have to notice that substituted alloy should not form single-phase solution as it is reported [42].

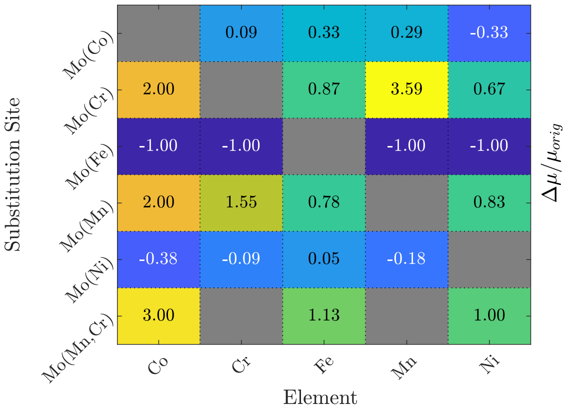

Figure 2: Relative change of atomic magnetic moment in the dependence of on the position of Mn doping.

3.2. Exchange interaction

Having the relation between a composition and a magnetic structure or magnetic moments we calculated the exchange interaction in the parent Cantor alloy and its derivatives (Figs. 3, 4) for both BCC and FCC lattice structure. We expected obtaining extra information to previously described behavior. In calculation the FM phases were mostly used. The exceptions were the Cantor alloy, where non-zero moments were found only in SDW case, FCC CoCrMoMnNi, which was excludes due to absence of a magnetism and MoCrFeMnNi alloy, where interaction for parallel spins in paramagnetic phase are depicted. Otherwise the FM phase is the ground state. We remind that we used scalar relativistic approach instead of fully relativistic one, due to an implementation of the Liechtenstein formula. Although it caused mostly suppression of magnetic moments, the properties almost weren't changed in general. There was only two significant difference. Primary in BCC CoCrMoMnNi alloy, where the directions and magnitudes were change and secondary for FCC CoCrFeMnMo, which was non-magnetic in the scalar relativistic approach.

The results showed, that the dominant interactions in FCC and BCC structure differers by one order of magnitude. It explains larger magnetic moments and tendency to FM ordering for a BCC structure. We can assume that the difference is caused by structural symmetry and not by volume effect, because the equilibrium lattice parameters refer to the same Wigner-Seitz radii for both structures. Exchange interactions in BCC structure are dominated by ferromagnetic interaction of Co, Fe and Mn atoms, which likewise poses the largest magnetic moments. Antiferromagnetic interaction are almost negligible there. There should be probably an exception for CoCrMoMnNi, but scalar-relativistic approach gives positive magnitudes of magnetic moments. The interactions of Cr and Ni atoms are even weaker and therefore we observed only smaller magnetic moments in different directions, which probably comes from interplay of comparable parallel and anti-parallel interactions. The DLM phase in case of MoCoFeMnNi should prevail due

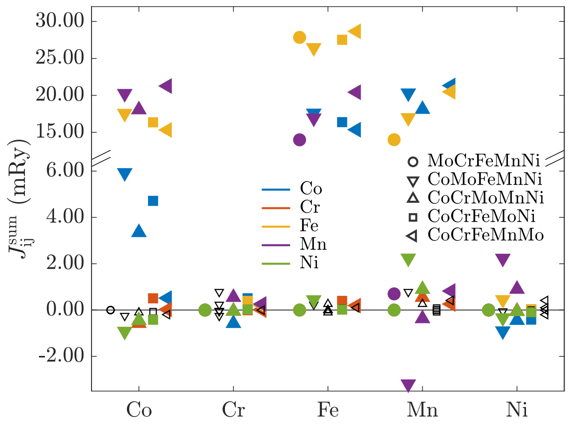

Figure 3: Sums of exchange interaction J_{ij} in BCC structure with resolved alloys and counterparts. The sum if over ten nearest neighbour shells. Unfilled point denotes interactions related to Mo atoms.

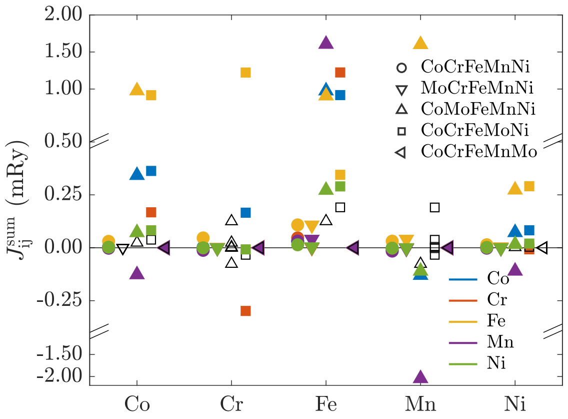

Figure 4: Sums of exchange interaction J_{ij} in FCC structure with resolved alloys and counterparts. The sum if over ten nearest neighbour shells. Unfilled point denotes interactions related to Mo atoms.

to the loss of strong ferromagnetic interaction originated related to Co atoms. Since then the magnetism rely only on diluted Fe atoms.

The situation in a FCC structure in much more complicated due to the non-existence of such dominant interactions as in the previous structure [43]. The most significant interaction are related to Fe atoms. Depending on the substitution interaction with Co, Cr and Mn become important. In comparison to the BCC chromium interactions seems to be more important for a magnetic behavior there. The fact that the most important interactions rely on Fe atoms confirms Fe importance for magnetic behavior stated above. Similarly Co related interaction still remain important and their loss leads to DLM state. It was observed, that interactions related to Cr and Mn atoms are strengthened if the counterpart element is absent. It manifests their mutual dislike in the system.

3.3. Varied concentration CoCrFeMnNi

In addition to studies using a substitution of an element in the parent alloy by the mom-magnetic molybdenum, we tried to study the importance of elements in the CoCrFeMnNi alloy by multilayer system with a varying concentration on the elements, where the total concentration was kept. Therefore the total energy can be easily compared due to the same total composition. We employ a SDW phase possessing the highest magnetic moment. In introduced SDW layer system based on FCC close packed structure one can easily vary the composition in each layer thank to the CPA. The number of layer is limited only by a computation demands. Further the effect of a changed concentration in a single layer should prevail over effect in the other layers compensating the change in the stoichiometry, where the perturbation spreads out. A four-layered system were chosen. In the first layer the concentration 0.05 0.10 and 0.30 for a selected element were used. We didn't simulate larger systems due to their time demands. We find that for the system with a glut of an element in the first layer the energy almost remain unchanged. Where as its lack cause large energetic differences. It was observed that the loss of Co or Ni atom is energetically disadvantageous. Lack of iron atom gives relatively small energetic gain.

A stabilization of the magnetic system by a lack manganese or even more chromium atoms confirms results obtained in calculation of Mo derivatives, where especially Mn and Cr substitution stabilize FM phase (Fig. 5). Further it correspond to the suppression of magnetic moments or magnetic interaction by Cr or Mn. The enhancing of magnetic moments in alloys lacking part of Cr or Mn atoms was observed also in the layered system, both in the first layer and in total. Besides there can be correspondence with reported enhancing melting temperature, while an amount on Mn is reduced [39]. Finally a significant role of Ni atom in a magnetic structure was revealed. Large energy differencies might leads to forming of precipitates lacking an element, but on the contrary they would have reduced formation entropy. Hence it is not if they appears there.

4. Conclusions

We have studied the magnetic properties of CoCrFeMnNi belonging to the high entropy alloys and its

magnetic structure	lattice	lattice parameter (Å)	magnetic moments per element (μ_{B})				
			CoCrFeMnNi				
SDW	FCC	3.48	0.05	-0.05	0.34	-0.07	0.02
			MoCrFeMnNi				
DLM	BCC	2.88	0.00	0.00	1.96	1.07	0.00
	FCC	3.62	0.00	0.00	0.74	-0.03	0.00
			CoMoFeMnNi				
FM	BCC	2.87	1.40	-0.22	2.22	1.97	0.28
	FCC	3.59	0.35	-0.05	1.43	-0.77	0.08
			CoCrMoMnNi				
FM	BCC	2.88	1.78	-0.13	-0.09	1.66	0.11
			CoCrFeMoNi				
FM	BCC	2.88	1.26	-0.04	2.14	-0.08	0.12
	FCC	3.61	0.36	-0.28	1.35	-0.08	0.08
			CoCrMoMnNi				
FM	BCC	2.88	1.38	-0.04	2.12	1.64	-0.11

Table 3: Calculated lattice parameters and magnetic moments for CoCrFeMnNi and its derivatives obtained within scalar relativistic method

derivatives formed by molybdenum substitution. Primary we showed a reliability of our method comparing obtained results to the published ones. Later a relation between presence of magnetic elements and ground state properties was discussed.

Using the nonmagnetic substitution of CoCrFeMnNi alloy we investigate the influence of the magnetism of its components to the stability of the alloy and the preferred magnetic phase. Calculation reveal a stabilization effect caused by the absence of Mn or Cr atoms. Not only does it decrease formation enthalpy as showed calculation of Mo-derivatives or layered CoCrFeMnNi systems, but it also shift the system to the magnetic state. Besides a crucial role of Fe and Co atoms for establish magnetism was observed. Finally the necessity of the Ni presence for system stability was discovered.

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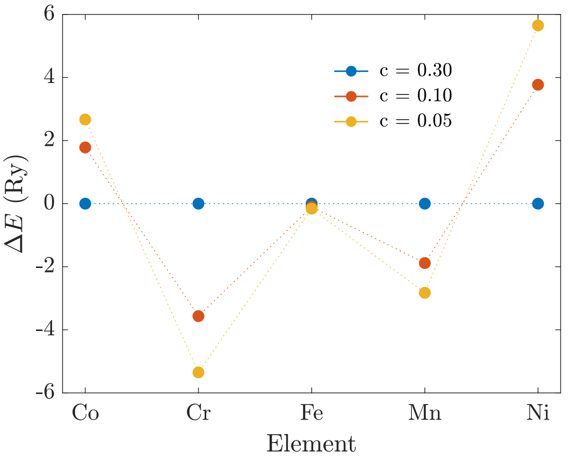

Figure 5: Dependence of the total energy on the selective change of concentrations of elements in a layered system, while the the total stoichiometry is preserved

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